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Numerical study of n-heptane and air mixture combustion inside a micro tube

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Abstract

A numerical study on n-heptane and air premixed combustion inside a micro tube is undertaken to investigate. The simulation result shows that the flame location moves towards downstream as the fuel mass rate improves and the rate of location and mass rate is $K_1=x/m_f$=14.22m • s/g, the product of temperature slope and mass rate is $P_t=S_t \bullet m_f$ =10.43K • g/m • s. With equivalence ratio's increasing, the flame moves upstream when mass rate is constant and temperature drops slowly first and then rapidly. The equivalence ratio can cut the combustion efficiency. A bigger heat loss rate h can make the temperature go down faster and cut the peak temperature a little.

Keywords: micro tube, n-heptane, fuel mass flow rate, equivalence ratio, heat loss rate

1. Introduction

In the past two decades, the combustion reaction in the micro and meso scale tube as a component of micro power system has been investigated intensively with the fast development of MEMS devices. Compared with the Li batteries, the micro-scale power system using hydrocarbons as fuel has significantly larger energy density, and has a very vast prospect [1].

The combustion in micro tube has less stable and more challenge than traditional ones. The large S/V ratio of micro tube leads to a severer heat-loss effect which cases the flame instability. The channel is usually closely related to the quenching diameter which has influence on the stabilization. The residence time of mixture gas in micro tube is so small for the complete reaction that the combustion efficiency is lower. For the macromolecular hydrocarbon, it has much more complex oxidation reaction, bigger quenching diameter, longer complete reaction time. The combustion of micromolecular fuels in micro

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tube is usually considered by the researchers. Liang Feng et al. numerical analyzed the methane and air premixed combustion inside a small tube with a temperature gradient at the wall [2]. Jianlong Wan et al. studied the combustion characteristics of lean hydrogen/air mixture in a planar micro-channel with a bluff body [3]. Jinsong Hua team and J. Li team separately investigated the hydrogen/oxygen mixture and the methane/oxygen mixture combustion in the micro tube with an expanding inlet, using the CFD software [4,5]. In this paper, the combustion of n-heptane in micro tube is numerical studied, and effect of various parameters on the temperature distribution and combustion efficiency are analyzed.

2. Model

The geometry of the micro tube used in this paper is shown in Fig. 1. The combustion length l, inner diameter r, and wall thickness d are defined in this figure. The origin of coordinates O is fixed at the centre of the inlet plane. The n-heptane/air mixture which is assumed to be complete premixed is injected into the tube on the left side and the after burning gas is exhausted on the right side. The mass flow rate of mixture is defined by the fuel mass flow rate (m_f) and equivalence ratio (ER). In this paper, l=80mm, r=2mm, d=1mm, the inner temperature is 1200K, and the pressure is 1atm. The surface temperature of pipe is assumed to be the same with local gas. The simulation of combustion is performed by use of the software CHEMKIN 4.1 in a plug flow reactor. The Lawrence Livermore National Laboratory (LLNL) reduced n-heptane mechanism is used. It consists of 159 species and 770 reactions [6]. This mechanism has been proved to be a correct description for the n-heptane oxidation reaction [7].

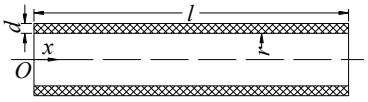

Fig. 1 Geometry model.

3. Results and discussion

3.1. Combustion characteristics

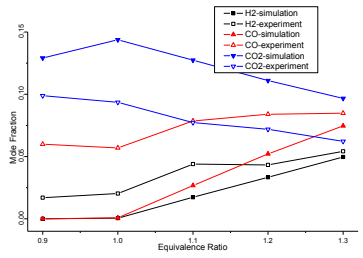

Fig. 2 Comparisons of H_2, CO and CO_2 between measured and computed compositions when ER=1.2 and m_f=0.45mg/s.

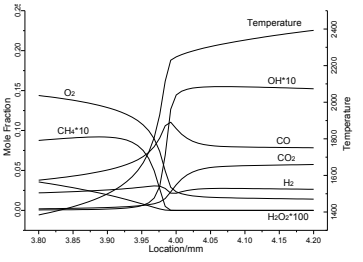

Fig. 3 Computed major species and temperature near the flame when ER=1.2 and m_f=0.45mg/s.

To validate the simulated result, the result is compared with that measured by the gas-chromatograph (Agilent 7890a) when m_f=0.45mg/s (Fig. 2). It can be found that the H_2, CO and CO_2 mole fractions measured by the both methods are similar and have the same trends. Fig. 3 shows the computed major species and temperature near the flame. Before the flame edge, the reaction releases a lot of energy which heats the gas and forms the flame. In the oxidation reaction of n-heptane, the fuel is consumed rapidly with producing a large amount of products and intermediate product, such as OH radical, H_2O_2, H_2 and CH_4 molecules. Most of the intermediates can not sustain long and the contents of them go down to zero

near the exhaust. At the downstream of flame, the products may be converted to one another, which are driven by the energy changing and temperature falling.

3.2. Effect of fuel mass flow rate

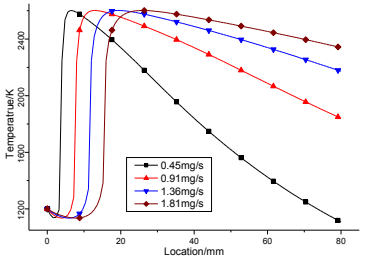

Fig. 4 Effect of fuel mass flow rate (m_f) on temperature when ER=1.2.

Fig. 4 shows the temperature distribution on the X axial. When ER is stable, the peak temperature stays the same, and the flame location goes downstream with m_f's increasing. It can be found that the flame location is in direct proportion to m_f and the relationship can be expressed as $K_T=x/m_f$=14.22m • s/g. At the downstream of flame, the temperature drops, with a faster rate of descent when m_f is huge. In fact, the product of temperature slope and m_f is constant, which can be also expressed as P_t =10.43K • g/m • s.

3.3. Effect of equivalence ratio

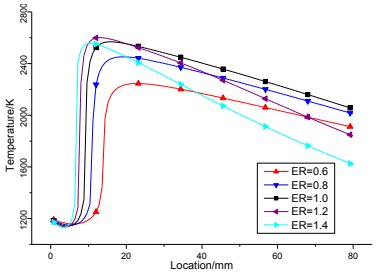

Fig. 5 Influence of equivalence ratio on temperature along the X axial when m_f=0.91mg/s

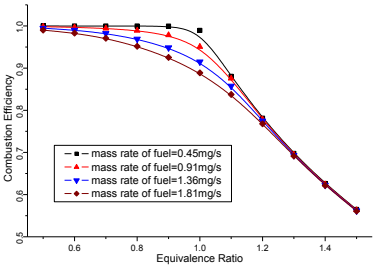

Fig. 6 Influence of equivalence ratio on combustion under various mass rate of fuel (m_f).

Fig. 5 shows the temperature along the X axial under various ERs. In a certain m_f, the location of the peak temperature (flame) moves towards upstream as the ER rises. But the temperature trends are different. When ER rises from 0.6 to 1.0, the temperature in the downstream of flame drops slower; and then it drops faster, which makes the exhaust temperature has the same rule with ER's increasing.

The effect of ER on combustion efficiency which is expressed as

$$\eta = 1 - \frac{\dot{m}_{H_2} LHV_{H_2} + \dot{m}_{CO} LHV_{CO}}{\dot{m}_{hep\tan e} LHV_{hep\tan e}}$$

is shown in Fig. 6. The reaction becomes more and more incomplete when ER is rising, and it drops from 1 to nearly 0.56. To be noticed, the efficiency changing law is different under various m_f. When m_f =0.45mg/s, the combustion efficiency changes a little (close to 1.00) while ER's rising to 1.0, and then it drops rapidly. When m_f is bigger, the efficiency is smaller and always drops with ER's increasing. The efficiency is almost the same when ER is bottom (0.5) and top (1.5) under different m_f. The increasing m_f can reduce the residence time of gas and decrease the efficiency.

3.4. Effect of heat loss

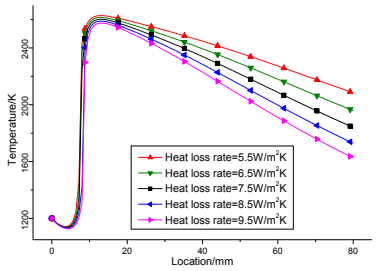

Fig. 7 Influence of heat loss rate on temperature when m_f=0.91mg/s and ER=1.2.

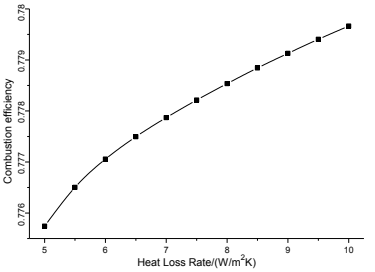

Fig. 8 Influence of heat loss rate on efficiency when m_f=0.91mg/s and ER=1.2.

The high temperature gas releases the energy to atmosphere through the wall and it drops (Fig. 7), which is determined by the heat loss rate (h). From the figure, the higher h is, the more heat loss per unit length is and the faster the temperature drops. At the exit of tube, the exhaust temperature when h=5.5 is 458℃ higher than that when h=9.5. The peak value of temperature in the micro tube is a little lower when h is huge. The reactions for product are mostly exothermic reaction. The dropping temperature caused by the heat loss is meaningful for the fuel conversion and improves the efficiency (Fig. 8).

Conclusion

The n-heptane/air mixture combustion in a micro tube is numerically investigated. The effects of the mass flow rate of fuel, the equivalence ratio and the heat loss rate are discussed in this paper:

1. The flame location moves towards downstream as m_f improves, with a direct proportion between them. The temperature goes down after the flame and the product of temperature slope and m_f is constant.
2. In a certain m_f, the flame moves upstream while ER is rising. The temperature drops slowly first and then rapidly. The combustion efficiency goes down when ER is higher.
3. A bigger heat loss rate h can make the temperature go down faster and the peak temperature is a little smaller. A serious heat loss will also improve the combustion efficiency.

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Biography

Jinghuai Huang, a PhD student in Beijing Institute of Technology. Over 4 years, Huang major in the micro combustion, Computational Fluid Dynamics and Chemical Reaction Kinetics of hydrocarbon fuel. Several papers are included in EI and SCI.